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EIGENVALUES OF SYMMETRIC FIVE-DIAGONAL MATRICES

by L. W. EHRLICH

THE JOHNS HOPKINS UNIVERSITY • APPLIED PHYSICS LABORATORY

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ABSTRACT

Several methods for finding eigenvalues of symmetric five-diagonal matrices are compared experimentally. The results indicate that if relatively few eigenvalues are desired a modified Sturm sequence and interpolation scheme is fastest.

CONTENTS

1. INTRODUCTION

We are concerned here with finding the lower (or higher) eigenvalues of symmetric, five-diagonal matrices. Several numerical techniques are experimentally compared, including one that uses a Sturm sequence-type approach directly on the five-diagonal matrix. The results indicate that if relatively few eigenvalues are desired a modified Sturm sequence and interpolation scheme is fastest.

2. LR TRANSFORMATION OF RUTISHAUSER (LR)

This method uses Cholesky decomposition with appropriate origin shift (Refs. 1 and 2, and Ref. 3, pp. 544-556). Each iteration requires 6n additions, 9n multiplications, 2n divisions, and n square roots. The method also requires a judicious choice of origin shift to be effective. A poor choice could invalidate the technique. The implementation used here was that of Ref. 2, which produces a cubically convergent technique. Since only a few eigenvalues are needed, we have O(n) operations. Although the Cholesky decomposition is used, the origin shift allows one to find eigenvalues of matrices that are not necessarily positive definite.

3. STURM SEQUENCE AND BISECTION (SS)

By the separation theorem, it is known that the eigenvalues of the (k-1)th leading principal minor, say A_{k-1}, of a symmetric matrix separate the eigenvalues of the kth leading principal minor, A_k, for each $k \le n$ (see, e.g., Ref. 3, p. 103). Thus, if we evaluate the leading principal minors of $(A-\lambda I)$, the number of variations in sign is the number of eigenvalues of A greater than λ.

Let

$$A = \begin{pmatrix} a_1 & b_2 & c_3 & & \\ b_2 & a_2 & b_3 & & 0 \\ c_3 & b_3 & a_3 & & \\ & & & & c_n \\ 0 & & & & b_n \\ & & c_n & b_n & a_n \end{pmatrix} .$$

In Ref. 4, Kuttler presented the following recurrence relation, where m_i is the ith principal minor:

$$\left.\begin{aligned} & m_{k-1} = q_k = 0, \qquad k \le 0 \\ & m_o = 1 \\ & q_{k-2} = b_{k-1}\, m_{k-3} - c_{k-1}\, q_{k-3} \\ & m_k = a_k m_{k-1} - b_k^2 m_{k-2} - c_k^2 (a_{k-1}\, m_{k-3} - c_{k-1}^2\, m_{k-4}) + 2 b_k c_k q_{k-2} \\ & \qquad k = 1, 2, \ldots, n \ . \end{aligned}\right\} \quad (1)$$

A count of the number of operations shows that we have roughly 10n multiplications and 5n additions, or 15n operations per iteration. It is necessary, however, to constantly scale the process to prevent underflow or overflow (see also comments at end of Section 6).

In Ref. 5 Sweet presents another set of recurrence relations to evaluate successive minor. However, simplifying his equations for a symmetric matrix, it turns out that one needs roughly 14n multiplications, 8n additions, and n divisions, or 23n operations per iteration, which is not competitive with the above.

4. STURM SEQUENCE AND INTERPOLATION (SSI)

In Ref. 6, a scheme is described whereby the number of bisections (and functional evaluations) may be reduced. Once bisection has isolated a single eigenvalue in some interval, an interpolation procedure is initiated. The procedure is attributed to Wyngaarden, Zonneveld, Dykstra, and Dekker, and its implementation is described in Ref. 6. Since the scheme requires a single eigenvalue to be isolated, one cannot find multiple eigenvalues by this method.

5. BAND DECOMPOSITION AND INTERPOLATION (BD)

In Ref. 7, a scheme is given whereby a band matrix is decomposed into its LU product with pivoting. If the matrix is symmetric and if $(A - \lambda I)$ is decomposed, one can determine the variations in the signs of the principal minors and thus use the approach of Section 4. Since the decomposition requires 7n additions, 7n multiplications, and 2n divisions or 16 n operations for a five-diagonal matrix, the method appears to be competitive with that of Section 3. We have not, however, taken into account the bookkeeping necessary for pivot determination, interchanging, etc.

6. MODIFIED STURM SEQUENCE (MSS)

In an effort to avoid the constant scaling of the Sturm sequence relation, we consider the approach used in Ref. 8. Let

$$M_k = \frac{m_k}{m_{k-1}} \quad , \qquad\qquad Q_{k-2} = \frac{q_{k-2}}{m_{k-1}} \quad .$$

Then Eq. (1) becomes

$$\left.\begin{aligned}
M_1 &= a_1 \\
M_2 &= a_2 - \frac{b_2^2}{M_1} \\
Q_1 &= \frac{b_2}{M_1 M_2} \\
M_3 &= a_3 - \frac{b_3^2}{M_2} + \frac{c_3^2\, a_2}{M_1 M_2} + 2b_3\, c_3\, Q_1 \\
Q_{k-2} &= \frac{b_{k-1}}{M_{k-1}\, M_{k-2}} - c_{k-1}\frac{Q_{k-3}}{M_{k-1}} \\
M_k &= a_k - \frac{b_k^2}{M_{k-1}} - \frac{c_k^2}{M_{k-1}\, M_{k-2}}\left(a_{k-1} - \frac{c_{k-1}^2}{M_{k-3}}\right) + 2b_k c_k Q_{k-2} \\
&\qquad\qquad k = 4, 5, \ldots, n \; .
\end{aligned}\right\} \quad (2)$$

However, it was pointed out to the author that this could be greatly simplified as follows:

$$
\begin{aligned}
&M_1 = a_1 \\
&P_2 = b_2 \\
&M_2 = a_2 - P_2^2/M_1 \\
&P_k = b_k - c_k P_{k-1}/M_{k-2} \\
&M_k = a_k - c_k^2/M_{k-2} - P_k^2/M_{k-1} \qquad k = 3, \ldots, n .
\end{aligned} \tag{3}
$$

where we identify

$$Q_{k-1} = P_k/(M_k M_{k-1}) .$$

This is equivalent to decomposing the matrix into its LU product, without pivoting. We need only count the number of $M_i < 0$. A count of the number of operations involved leads to 2n multiplications, 3n additions, and 3n divisions, or about 8n operations with no scaling. Unquestionably, this is the fastest method, but the lack of pivoting introduces a question of accuracy.

If the interpolation method of Section 4 is to be used (SSI), we must compute $\prod_{i=1}^{n} M_i$ for the functional values. It is somewhat simpler to scale this running produc than to scale the recurrence process (Eq. (1)).

The implementation of Eq. (3) was done in a manner similar to that described in Ref. 8. A test was made to determine if M_i vanished and, if so, to replace the zero with a relatively small number. This never occurred in any of the matrices tested. Also, unlike the Sturm sequence technique for tridiagonal matrices, it is not easy to see the conditions under which two successive M_i (or m_i in Eq. (1)) vanish. A check was made to determine if this happened and, if so, to perturb λ and try again. However, the situation never arose.

7. JACOBI ROTATIONS TO TRIDIAGONAL MATRIX (RJ)

If all eigenvalues are desired, we can, of course, use any of the above methods. However, there is an approach available in this case that is not competitive if only a few eigenvalues are desired. This is the method of Jacobi rotations to reduce the bandwidth of a matrix but preserve the band nature of the matrix, as suggested by Rutishauser (Ref. 9) (see also Ref. 10), followed by finding the eigenvalues of the resulting tridiagonal matrix by the QR method (Ref. 11).

8. RESULTS

For test matrices we consider the following:

$$A = \begin{pmatrix} p-r & 2q & r & & & \\ 2q & p & 2q & r & & \\ r & 2q & p & 2q & r & \\ & & & & & \\ & & & & & r \\ & & & & p & 2q \\ & & & r & 2q & p-r \end{pmatrix}_{n\times n} .$$

The eigenvalues of this matrix are

$$\lambda_k = (p-2r) - \frac{1}{r}(q^2-(q-2r\cos k\theta)^2)$$

$$= p - 2r - 4(q\cos k\theta - r\cos^2 k\theta)\,, \quad \theta = \frac{\pi}{n+1}$$

$$= p - 4q\cos k\theta + 2r\cos 2\,k\theta\,, \quad k=1,2,\ldots,n$$

(see, e.g., Ref. 12). In particular we chose four matrices, as follows:

Matrix 1:	$p = 7$,	$q = 1.75$,	$r = 0.4$
Matrix 2:	$p = 6$,	$q = 1.75$,	$r = 0.5$
Matrix 3:	$p = 11$,	$q = 10^{-15}$,	$r = 5$
Matrix 4:	$p = 10$,	$q = 10^{-15}$,	$r = 5$.

For matrices 1 and 2, the eigenvalues are distinct but of the smaller ones, many are near 1 for matrix 1, and near 0 for matrix 2. For matrices 3 and 4 each root is at least a double root (for even n) to within the precision of the arithmetic used, with distributions similar to matrices 1 and 2, respectively.

For computing only a few eigenvalues we used the methods of Sections 2, 5, and 6. For computing all eigenvalues, we compare the best of the above methods with the method of Section 7.

Each of these methods was applied in double precision in Fortran IV (H compiler) on the IBM 360/91 at The Johns Hopkins University Applied Physics Laboratory. Tables 1 and 2 contain the central processing unit (CPU) time in seconds for each run. Because of the time-sharing capabilities of the machine, it is possible that two identical runs could show slightly different times. However, the relative magnitudes of the numbers are consistent, and it is these in which we are interested.

In Table 1, the time is given in which the ten smallest eigenvalues were found. As noted above, methods BD and MSSI are identical except that the Sturm sequence process is determined by LU decomposition with pivoting in one case (BD), and without pivoting in the other (MSSI). Operation count indicates that BD should take about twice as long as MSSI, but the actual figure was between six and seven times as long. This was probably because of the work needed to determine and execute the pivoting. Also examination of the eigenvalues of the matrices up to order 2000 showed no difference in the accuracy of the two methods.

In Table 2, we have the time in seconds to compute all eigenvalues. For a given tridiagonal matrix, the QR method is fastest. We have included the QD method (Ref. 13) for comparison. It would seem that the QR method could be used even when only a few eigenvalues are needed. Unfortunately, "the order in which the eigenvalues are

Table 1

CPU Time in Seconds to Compute Ten Smallest Eigenvalues

Matrix		1	2	3	4
	BD	6.772	6.823	9.325	9.595
N = 500	LR	2.877	2.337	1.986	1.469
	MSS	2.502	2.590	1.374	1.384
	MSSI	1.134	1.195	1.364	1.383
	BD	13.655	13.760	17.955	18.402
N = 1000	LR	5.887	4.629	4.196	3.013
	MSS	4.851	4.913	2.610	2.760
	MSSI	2.230	2.252	2.675	2.750
	LR	12.458	9.673	8.491	5.785
N = 2000	MSS	9.223	9.519	5.139	5.298
	MSSI	4.380	4.412	4.937	5.071
N = 5000	MSSI	10.751	10.817	11.773	12.087

Table 2

CPU Time in Seconds to Compute all Eigenvalues

	Matrix 1			Matrix 4		
N	100	200	500	100	200	500
LR	1.969	7.278		1.311	4.935	
MSSI	1.835	7.277		2.818	11.108	
RJ only	0.156	0.627	3.969	0.156	0.636	4.081
RJ + QD	0.629	2.673	17.097	1.259	5.086	31.603
RJ + QR	0.445	1.693	10.2[illegible]4	0.381	1.523	9.348

found is to some extent arbitrary" (Ref. 11). The QD method, however, has the advantage of producing the eigenvalues in strictly ascending order. A comparison of Tables 1 and 2 shows that the QD method might be competitive if more than a few, but not all, eigenvalues are desired.

9. CONCLUSIONS

If only a few eigenvalues of a large five-diagonal symmetric matrix are wanted, the modified Sturm sequence and interpolation technique (MSSI) appears optimal. If all eigenvalues are desired, Jacobi rotations, followed by the QR method, appear difficult to beat. Between these extremes one might consider the LR or QD methods.

REFERENCES

1. H. Rutishauser, "Solution of Eigenvalue Problems with the LR-Transformation," National Bureau of Standards, AMS, Vol. 49, 1958, pp. 47-81.

2. H. Rutishauser and H. R. Schwarz, "The LR Transformation Method for Symmetric Matrices," Numerische Mathematik, Vol. 5, 1963, pp. 273-289.

3. J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

4. J. R. Kuttler, "Upper and Lower Bounds for Eigenvalues of Torsion and Bending Problems by Finite Difference Methods," ZAMP, Vol. 21, 1970, pp. 326-342.

5. R. A. Sweet, "A Recursive Relation for the Determinant of a Pentadiagonal Matrix," Comm. of the ACM, Vol. 12, 1962, pp. 330-332.

6. G. Peters and J. H. Wilkinson, "Eigenvalues of $Ax = \lambda Bx$ with Band Symmetric A and B," Comp. Jr., Vol. 12, 1969, pp. 398-404.

7. R. S. Martin and J. H. Wilkinson, "Solution of Symmetric and Unsymmetric Band Equations and the Calculation of Eigenvectors of Band Matrices," Numerische Mathematik, Vol. 9, 1967, pp. 279-301.

8. W. Barth, R. S. Martin, and J. H. Wilkinson, "Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection," Numerische Mathematik, Vol. 9, 1967, pp. 386-393.

9. H. Rutishauser, "On Jacobi Rotation Patterns," Proceedings AMS Symposium in Applied Mathematics, Vol. 15, 1963, pp. 219-239.

10. H. R. Schwarz, "Tridiagonalization of a Symmetric Band Matrix," Numerische Mathematik, Vol. 12, 1968, pp. 231-241.

11. H. Bowdler, R. S. Martin, C. Reinsch, and J. H. Wilkinson, "The QR and QL Algorithms for Symmetric Matrices," Numerische Mathematik, Vol. 11, 1968, pp. 293-306.

12. I. Galligani, A Comparison of Methods for Computing the Eigenvalues and Eigenvectors of a Matrix, Joint Nuclear Research Center, Ispra Establishment, Italy, 1968.

13. C. Reinsch and F. L. Bauer, "Rational QR Transformation with Newton Shift for Symmetric Tridiagonal Matrices," Numerische Mathematik, Vol. 11, 1968, pp. 264-272.